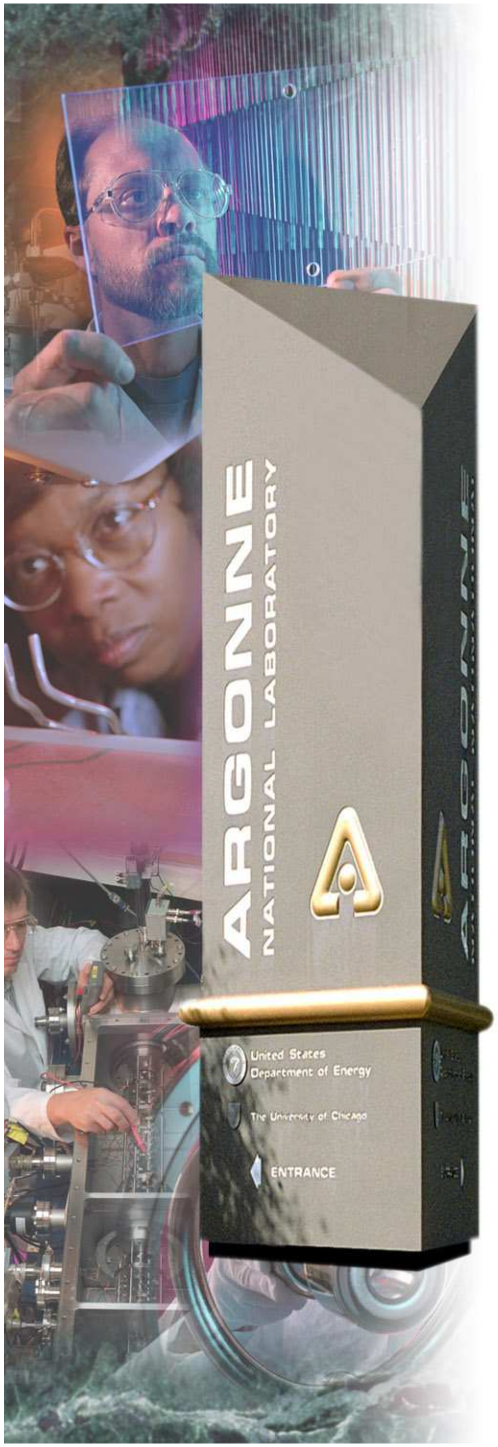

Argonne Fusion Work FY2006

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Office of Science
U.S. Department of Energy

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Outline

1. Erosion/Redeposition
2. Transients Simulation
3. MD Simulation
4. IMPACT Work

Fusion Personnel:

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Martin Nieto

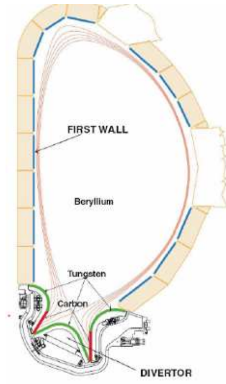
1. Erosion/Redeposition Modeling

- Continue analysis of ITER mixed material (Be/C/W) Plasma Facing Component performance. (ANL, LLNL, SNL)

- Perform updated analysis of NSTX MODULE-A performance and interpretation of results (ANL, LLNL, ORNL, PPPL)

- Continue PISCES/ITER beryllium/carbon mixed-material experiments modeling. (ANL, UCSD)

Continue analysis of mixed material PFC performance for ITER



ISSUES

- ***Lifetime*** *of* ***first wall*** *beryllium coating due to sputtering erosion.*
- ***Lifetime*** *of carbon (tungsten)* ***divertor*** *with mixed material (Be/C) sputtering/transport.*
- ***Tritium codeposition*** *in deposited carbon and beryllium.*
- ***Plasma contamination*** *by divertor and wall sputtering.*

Method: Package-OMEGA Analysis

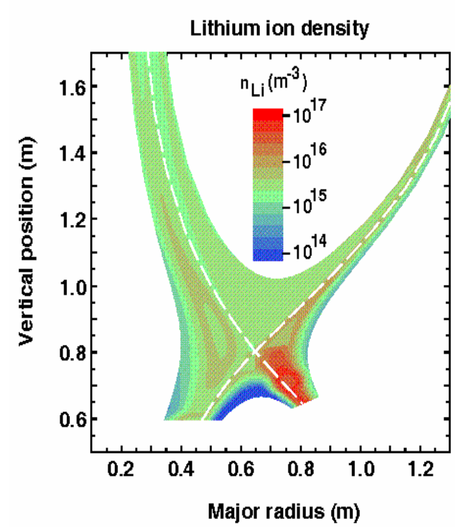
1) Compute sputtering of ITER beryllium wall with and without plasma convective flux to wall. (FY05)

2) Compute transport of sputtered beryllium to wall, divertor, plasma. (FY05)

3) Mixed material code analysis of Be/C mixing/sputtering on the ITER vertical divertor target.(FY06)

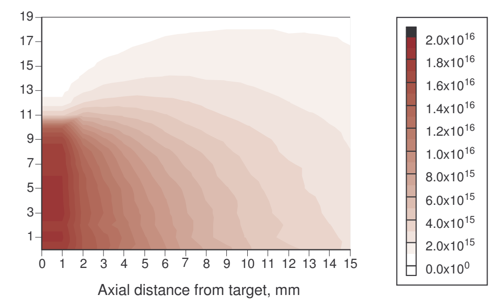
4) Compute erosion/redeposition, and surface-temperature dependent tritium codeposition in resulting growth layers of beryllium and carbon with inputs of oxygen flux to divertor and Q/Be and Q/Be-O codeposition rates. (FY06)

- **Perform updated analysis of NSTX MODULE-A performance and interpretation of results**
  - Purpose: Guide and interpret NSTX experiments.
  - Analysis will use updated models/data for thermal response of surface (with carbon and metal substrates), lithium sputter yields (data, MD, ITMC, TRIM, etc,. codes), plasma edge regime (UEDGE).



NSTX MOD-A Initial Li in plasma analysis

- **Continue PISCES/ITER beryllium/carbon mixed-material experiments modeling. (ANL, UCSD)**
  - Purpose: Validate mixed-material erosion/redeposition models for ITER predictive capability.
  - Analysis will focus on mixed Be/C sputtering, transport, and surface growth/mixing, code/data comparisons.



PISCES-REDEP Be-I density, Be/C experiment

2. Transient Analysis

(1) ELM Response:

- Integrated analysis and upgrade models of energy transport from core → SOL → PFCs
- Mixed material effects
- Sputtering during ELMs

(2) Disruption Effect

- Vaporization
- Melt splashing and erosion
- Brittle destruction of CBMs
- Mixed material effects
- *Mitigation!*

(3) VDEs

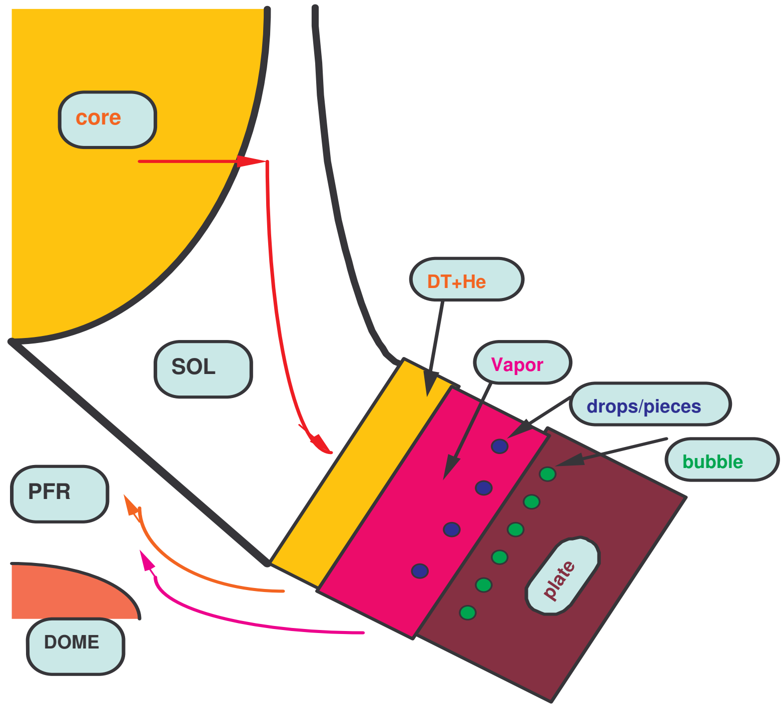
- Vaporization
- Melt splashing and erosion
- Brittle destruction of CBMs
- Mixed material effects

PLASMA

1. SOL dynamics
2. Interacaion with plate
3 Cloud dynamics
4. Droplets dynamics
5. Diffusion into core and PFR

DIVERTOR

5. Heat propagation
6. Melting and vaporization
7. Splashing / brittle destruction



Physical processes determining erosion/contamination problems

Pioneering Science and Technology

Ahmed Hassanein
PFC Meeting
Princeton Plasma Physics Laboratory
May 9-11, 2005

Office of Science
U.S. Department of Energy

Particle Transport Details

1. Energy/particle flux from core plasma to the SOL.

2. Energy/particle flux from SOL to PFC (divertor, wall, …)

3. Interaction of incoming ions (core particles - D, T, impurities) and electrons with divertor surface and vapor cloud above surface and resulting net absorbed energy.

4. Vaporization and sputtering losses.

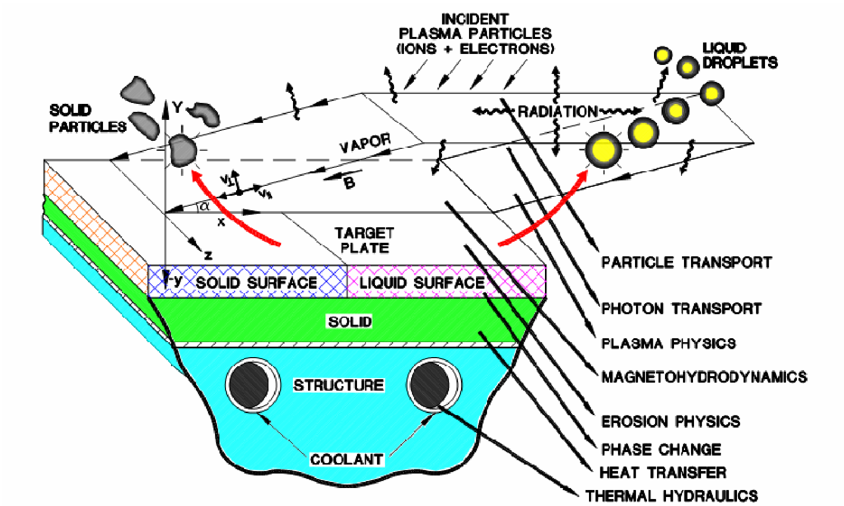
6. Melting and possible splashing in form of liquid metal droplets.

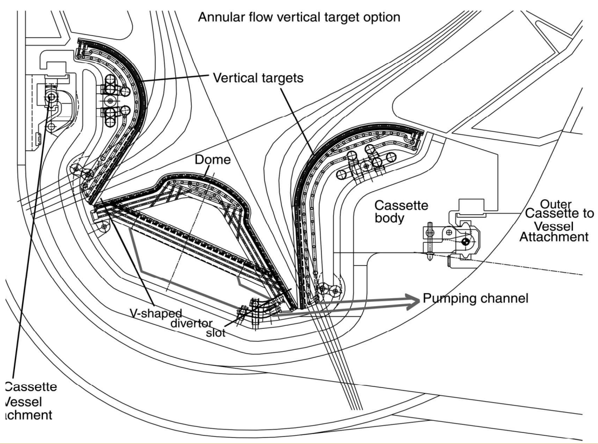
7. Motion of formed multicomponent plasma cloud (vapor + core particles stopped in cloud) in strong inclined magnetic field.

8. Noble gases for mitigations!

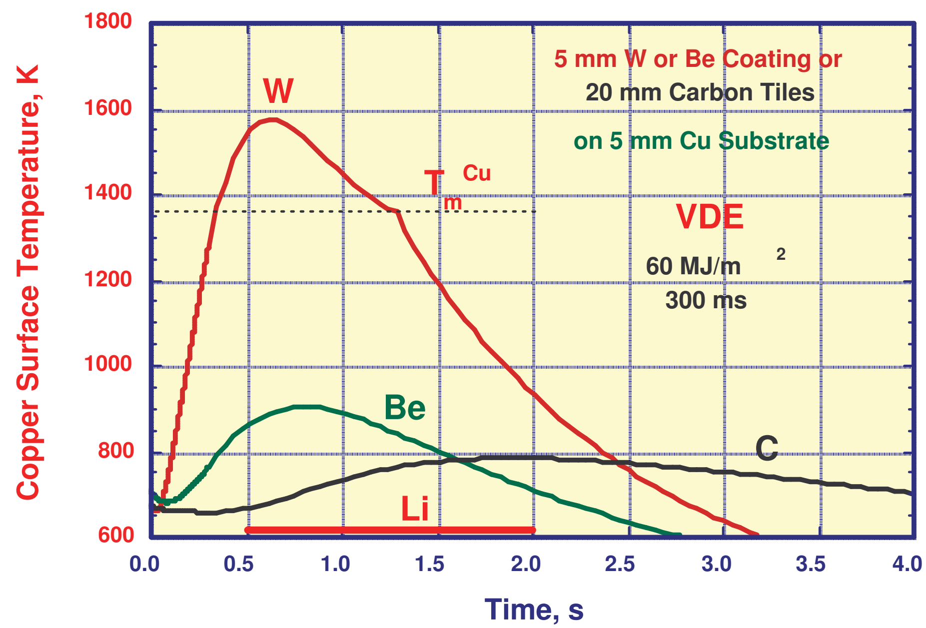
Radiation & VDE Analysis

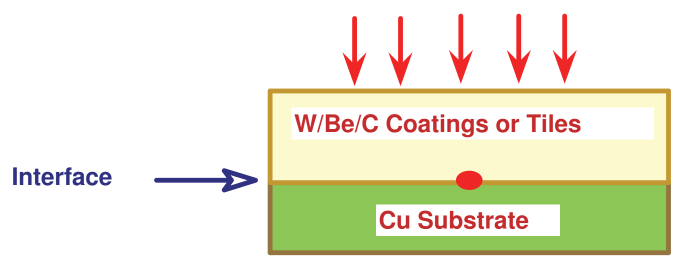
(2) Disruptions





(3) VDEs





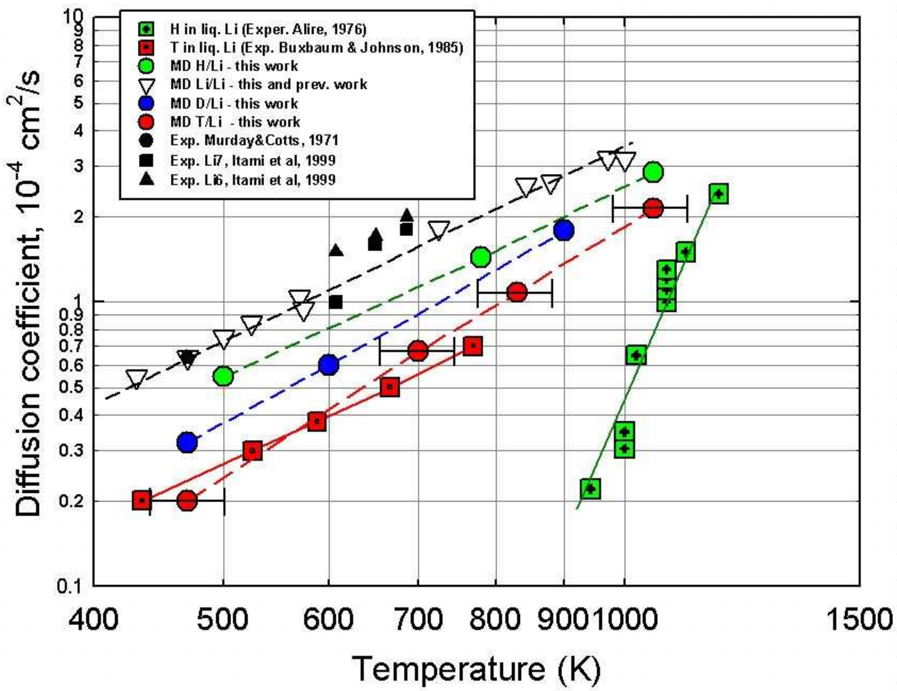
HEIGHTS Benchmarking & Collaborations

- Benchmark and collaboration with NSTX (PFC response)
- Benchmark with DIII-D (ELM physics)
- Benchmark with plasma gun devices (Erosion and Splashing):
  - QSPA TRINITI, Russia
  - QSPA Kh-50, Ukraine
  - MK-200, TRINITI, Russia
- Benchmark and collaboration with JUDITH, Germany (Brittle destruction of CBMs).
- Benchmark and collaboration with UIUC, plasma gun (physics/erosion?)

3. Molecular Dynamics for ITER

Diffusion retention of hydrogen and helium in prospective alloy first walls – e.g. W, Be, Carbon

MD is a powerful technique for the simulation of ion interaction with various surfaces. The figure below shows the results of the diffusion characteristics of hydrogen and helium in liquid lithium obtained in our MD work.



- We are developing a MD code for the simulation of pure and mixed W, Be and Carbon materials with and without hydrogen and helium effects
- Various inter-ionic potential functions will be developed and tested.
- Verification of the MD models are established by calculation of the H,D,T and self-diffusion coefficients and comparison with the available experimental data.

Bubble/Blister Formation in Metals

The bubble and blister formation effect in metals will further be studied

The atomistic simulation methods, such as Monte Carlo and MD, combined with the cluster formation kinetic theory are capable of understanding the thermodynamics and kinetics of the bubble formation in metals under a high hydrogen, helium irradiation flux.

This requires lots of work calculating the probabilities of association, dissociation, excitation and stabilization of small clusters of bubbles.

Bubble mass action law (Saha equations)

$A_2 \Leftrightarrow A + A$
$A_3 \Leftrightarrow A_2 + A$
…………..
$A_k \Leftrightarrow A_{k-1} + A \; \Sigma A_k = const\ (x,t)$

$$\begin{cases} n_2 \Leftrightarrow 2n_1 \\ n_3 \Leftrightarrow n_2 + n_1 \\ n_k \Leftrightarrow n_{k-1} + n_1 \\ \sum_{k=1}^{N} k n_k = n_{av}(\phi_{He}, T_{Li}) \end{cases}$$

$$n_k = n_{k-1} n_1 \left(\frac{2\pi\hbar^2 k}{m_1 k_B T} \right)^{3/2} \frac{Q_k}{Q_{k-1} Q_1} \exp\left(\beta\varepsilon_k - \beta\varepsilon_{k-1}\right),$$

$$Q_k = \sum_k g_k \exp\left(-\frac{E_k}{k_B T}\right) - \text{internal partition functions,}$$

ε_k – the binding energies for the cluster of k-atoms,

g_k – degeneracy of energy levels,

m_1 – He atomic mass, $\beta = 1/k_B T$

Kinetics of bubble formation

The kinetics of bubble (cluster) formation effects is a long studied subject in various areas. The Mean-field rate equations offer a complete obtaining concentrations of the bubbles (clusters).

$$\begin{cases} \dot{n}_1 = \Phi(z,t) - 2D\sigma_1 n_1^2 - 2D \sum_{s>1} \sigma_1 n_1^2, \\ \dot{n}_s = D n_1 \sum_{s>1} (\sigma_{s-1} n_{s-1} - \sigma_s n_s) - n_s \exp(-E_s / kT) \end{cases}$$

n_1 – the density of He atoms,

n_s – the density of bubbles with s (s >> 1) atoms,

$\Phi(z,t)$ – Helium flux from plasma,

D – Helium diffusion coefficient,

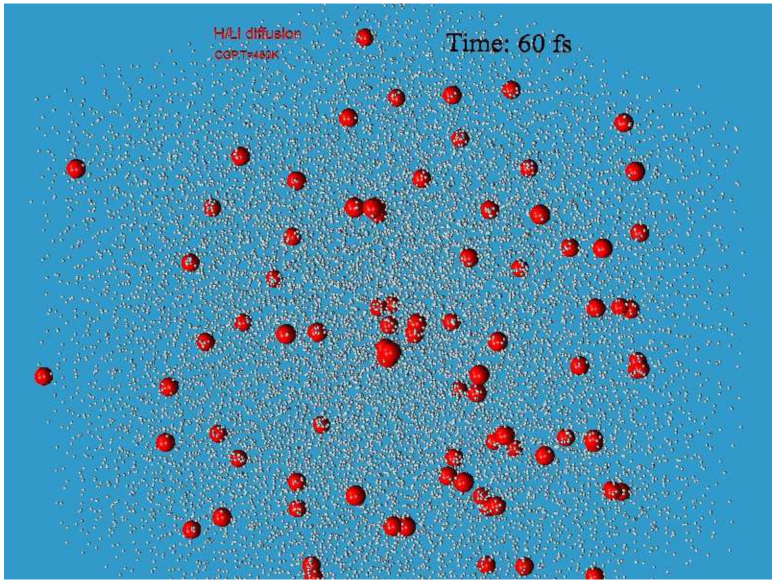
σ_s – capture probabilities,

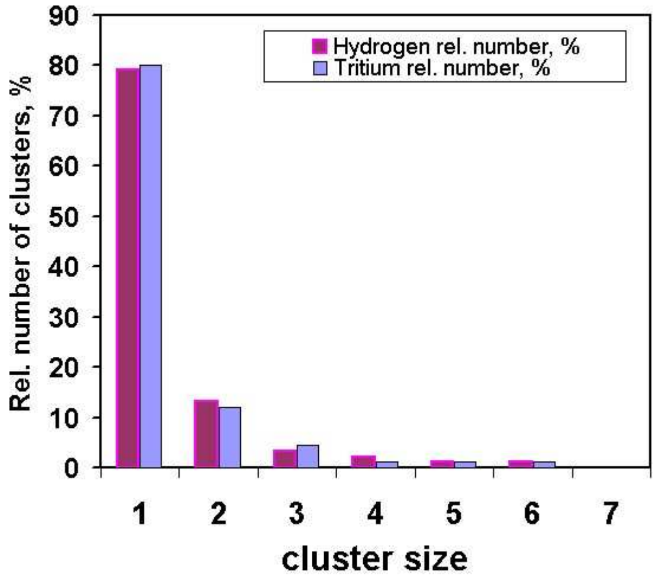
E_s – binding energy of a bubble with s atoms.

Splashing and shock waves

The dynamics of bubble formation will be studied by the direct MD simulation of surface tension, curvature radius, and Gibbs energy of the bubble

We have predicted that bubble formation in liquids (melted surfaces) during transient starts with the formation of small under-critical clusters which could significantly reduce the diffusivity of hydrogen and helium and increase the possibility of retention.



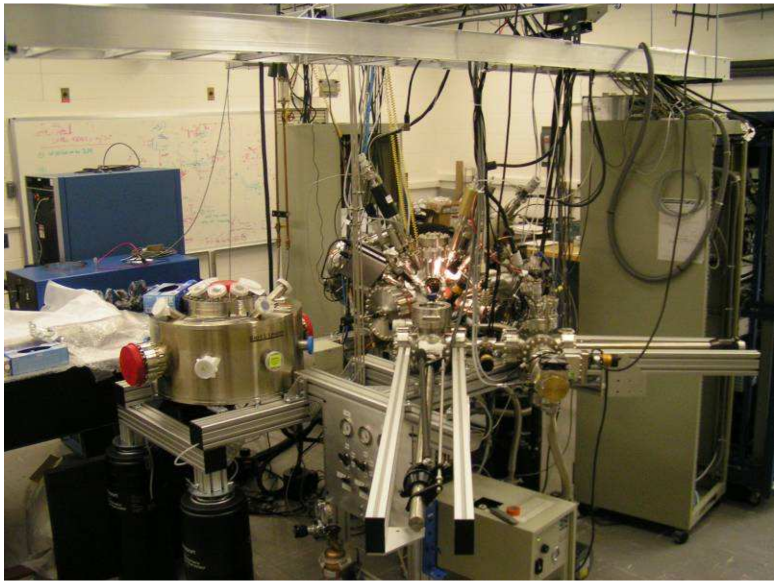


We have obtained preliminary results on bubble explosion and are planning to continue this work in the future.

4. IMPACT studies of plasma interactions with mixed-surfaces

- **Proposed mixed-material work in IMPACT will focus on ITER-related issues, namely:**
  - Study of hydrocarbon (e.g. C_xD_y) evolution for C-Be and C-W systems under near-threshold (5-100 eV/amu) energies at high temperatures 200-1000 °C.
  - Understand the role of oxygen on D-recycling properties and erosion levels of Be-based mixed surfaces (Be-C and Be-W).
  - Use of laser post-ionization TOF-MS in IMPACT to measure sputtered and molecular emission energy distributions.
- **Experiments will study the role of lithiated graphite surfaces:**
  - Hydrocarbon evolution under D^+ and He^+ bombardment
  - Physical sputtering of carbon under D, He and Li bombardment
- **Additional lithium thin-film work on alternate substrates**
  - Understand erosion and D-retention properties of Li thin-films on various substrates (Mo, W and SS) as function of ion bombardment and temperature. (supporting both NSTX and LTX missions).

IMPACT (Interactions of Materials with charged Particles and Components Testing) Experiment at Argonne



- IMPACT experiment is designed to study multi-functional and multi-component surfaces and interfaces under extreme particle irradiation conditions.
- IMPACT consists of in-situ metrology that allow for the time-dependent measurement of: surface evolution, surface erosion and eroded particle energy distributions while being modified by energetic particle bombardment.

IMPACT in-situ metrology

EUV source: EUPS

Multiple ion sources: ion-induced mechanisms
Surface analysis: LEISS, DRS

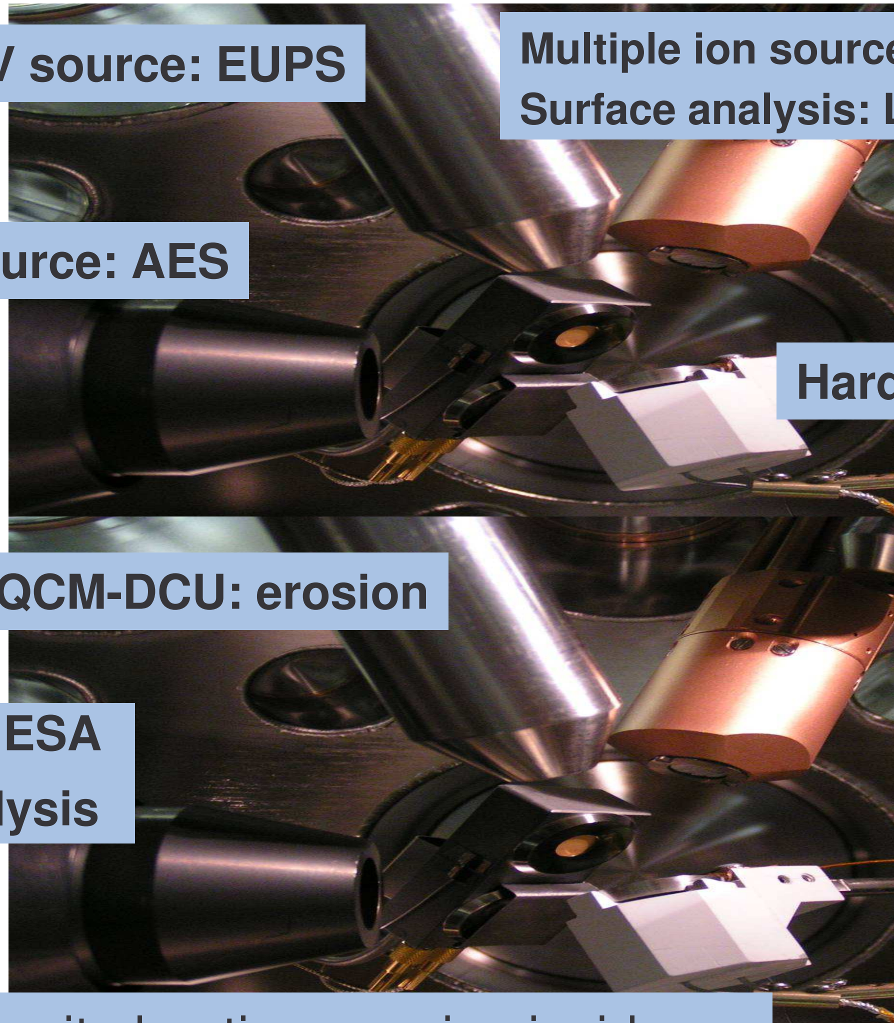
Electron source: AES

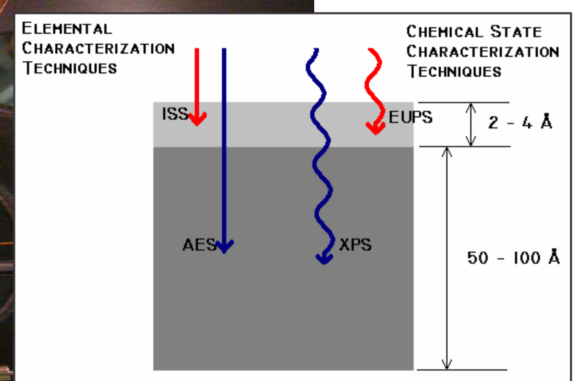
Hard X-ray source: XPS

Laser PI-SNMS

QCM-DCU: erosion

PHOIBOS HESA
Energy analysis





In-situ heating, grazing incidence

Complete diagnosis of a multi-component surface under irradiation